

2-Chloroethanol
107-07-3 | DTXSID1021877

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 6.87 mmHg

Global applicability domain: Inside

Local applicability domain index: 7.47e-01

Confidence level: 8.64e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>1,2-Dichloroethane</div> <div>Measured: 7.18</div> <div>Predicted: 99.3</div>	<div>Image not found</div> <div>2,3-Dichloro-1-propene</div> <div>Measured: 5.25</div> <div>Predicted: 61.5</div>	<div>Image not found</div> <div>Chloroprene</div> <div>Measured: 4.90</div> <div>Predicted: 175</div>
<div>Image not found</div> <div>Ethylenediamine</div> <div>Measured: 26.1</div> <div>Predicted: 6.61</div>	<div>Image not found</div> <div>2-Methylpent-1-ene</div> <div>Measured: 3.55</div> <div>Predicted: 61.0</div>	